Indirect solvent assisted tautomerism in 4-substituted phthalimide 2-hydroxy-Schiff bases

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1. NMR spectra

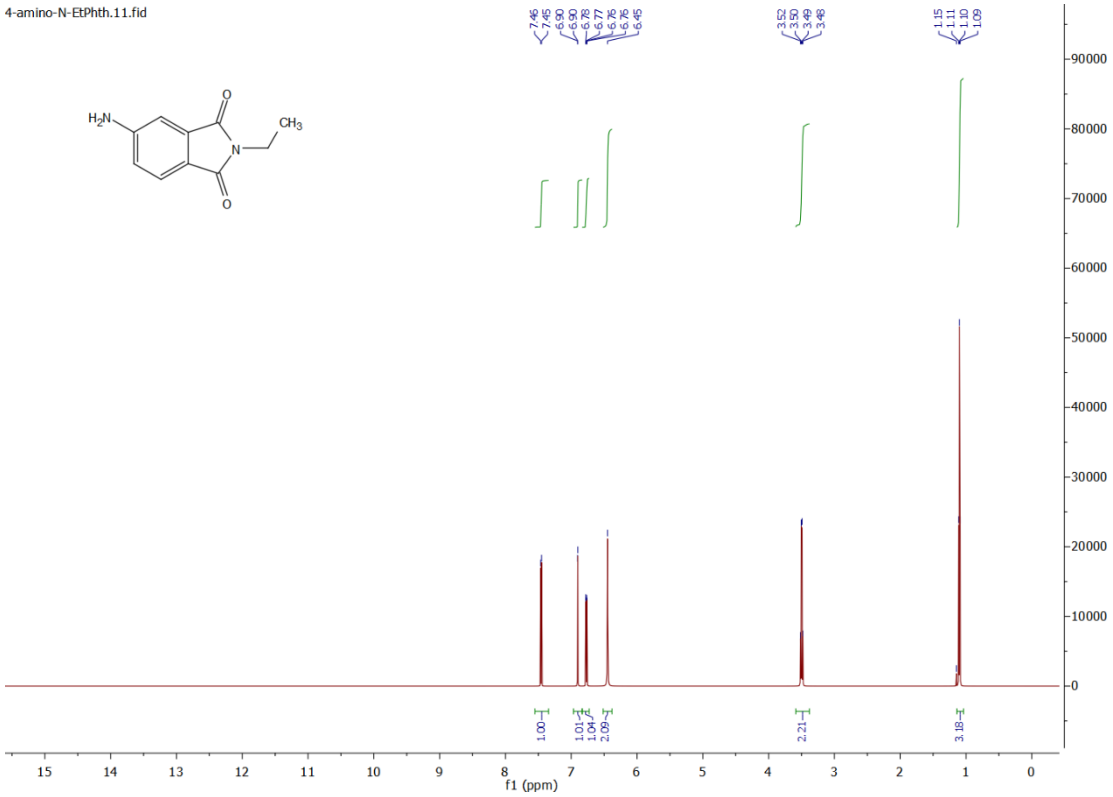


*Fig. S1.[1]H-NMR spectrum of **3** (4-amino-N-ethylphthalimide).*

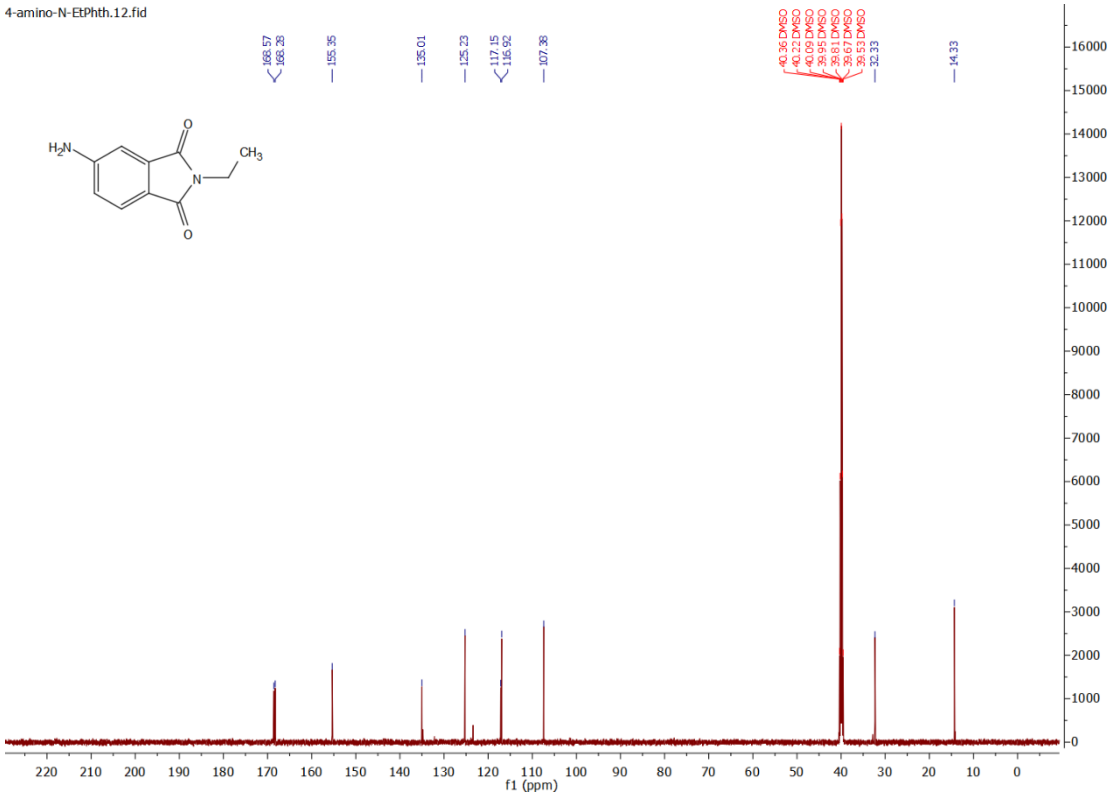


*Fig. S2.[13]C-NMR spectrum of **3** (4-amino-N-ethylphthalimide).*

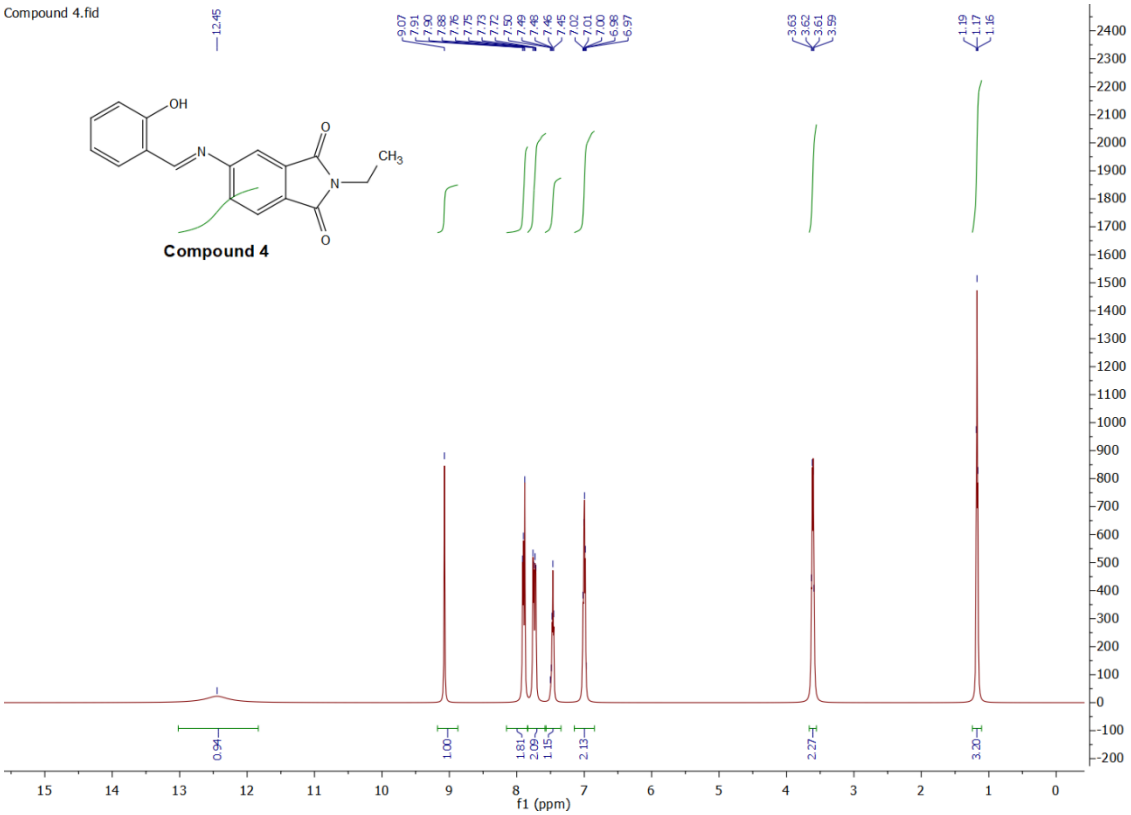


*Fig. S3.[1]H-NMR spectrum of **4***

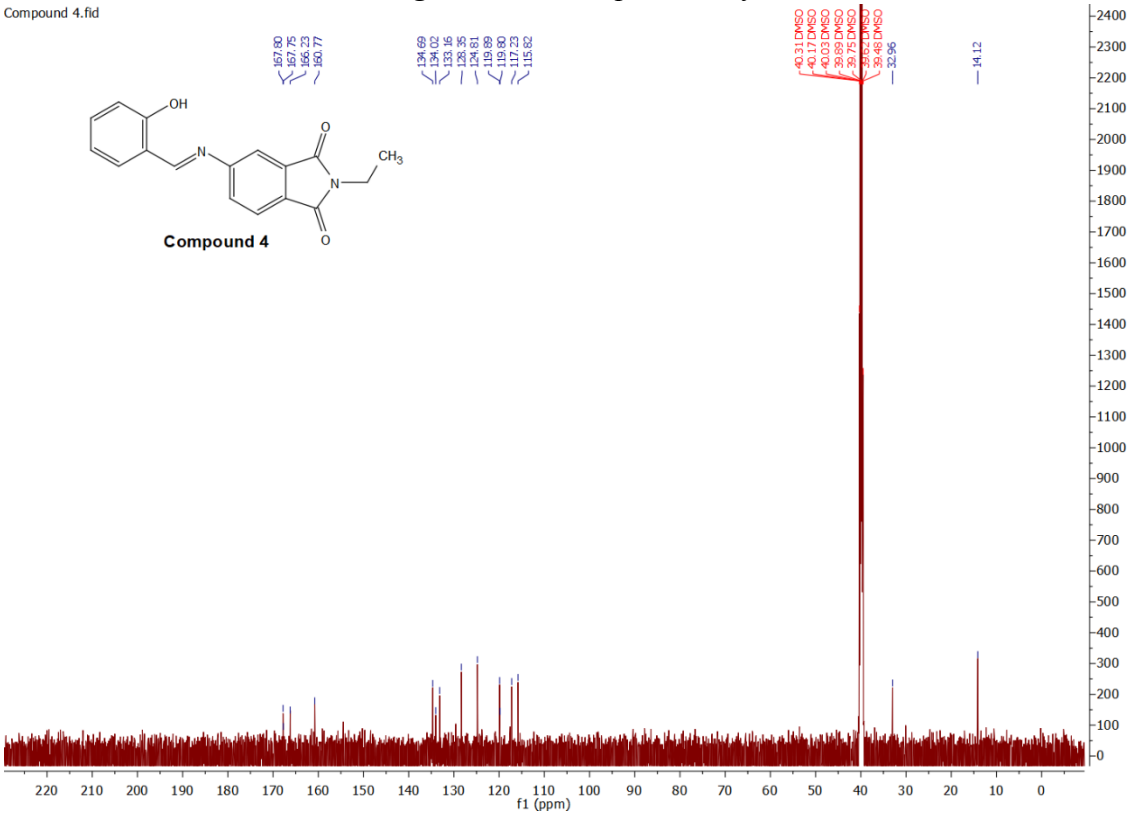


*Fig. S4.[13]C-NMR spectrum of **4***

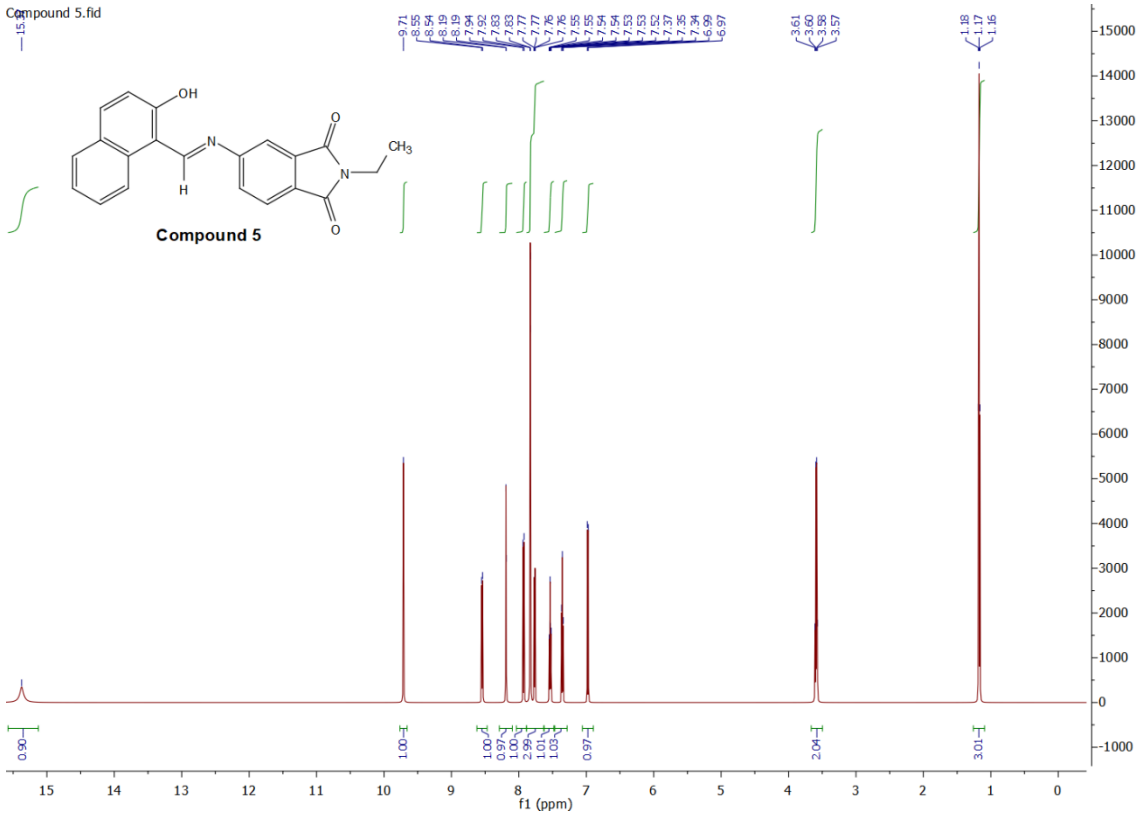


*Fig. S5.[1]H-NMR spectrum of **5***

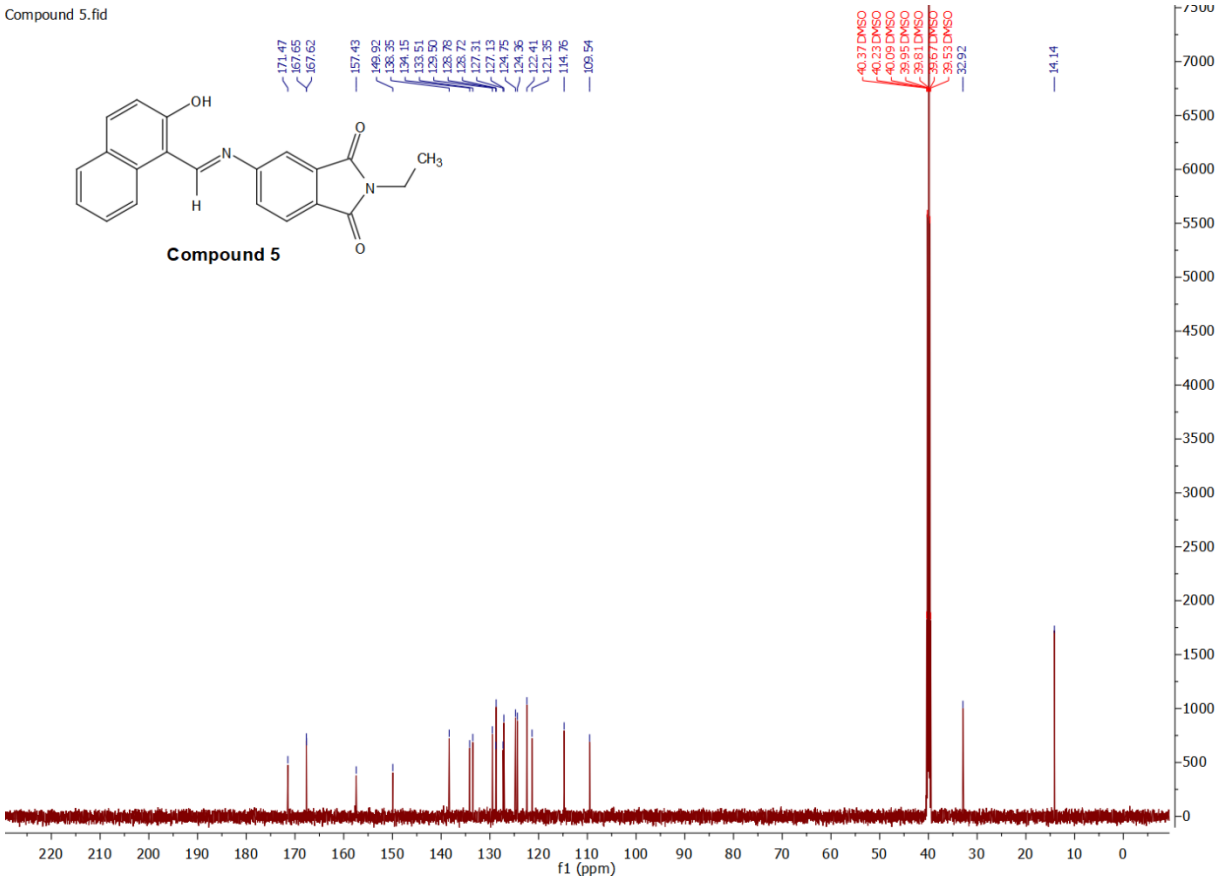


*Fig. S6.[13]C-NMR spectrum of **5***

2. ATR-IR spectra

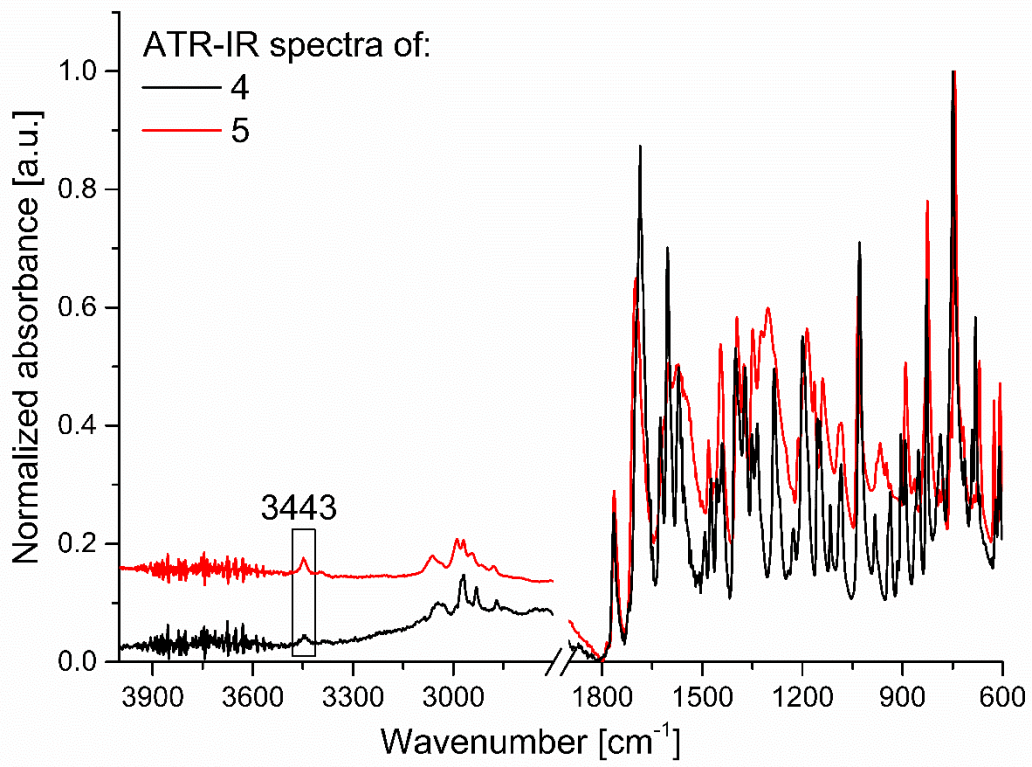
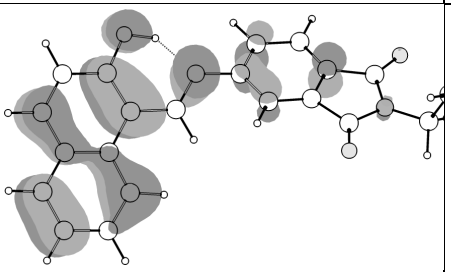
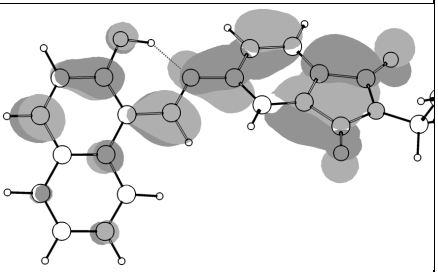
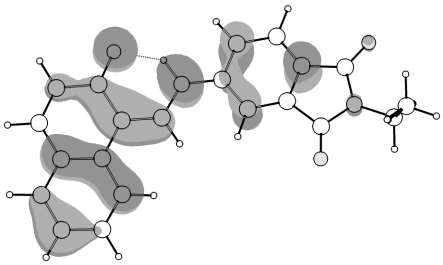
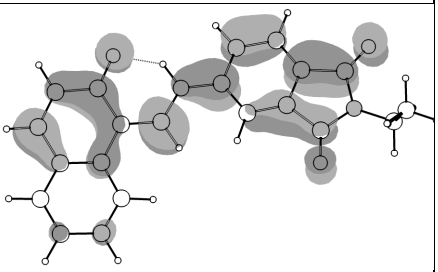
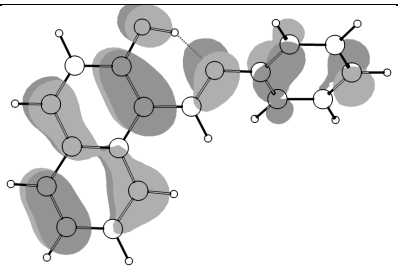
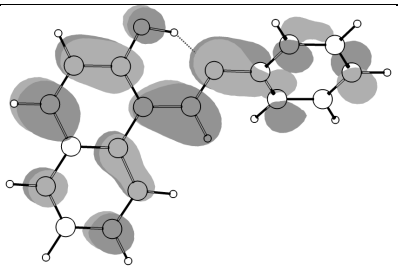
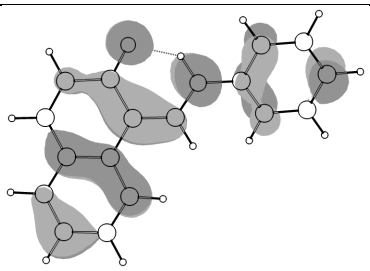
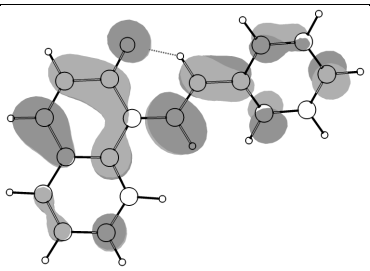


*Fig. S7. ATR-IR spectra of **4** and **5** as solids.*

3. HOMO and LUMO molecular orbitals

Table S1. HOMO and LUMO molecular orbitals of **5** and **6** in the gas phase.

Comp	Form	HOMO	LUMO
5	**E**		
	K		
6	**E**		
	K		

4. Fluorescence spectra

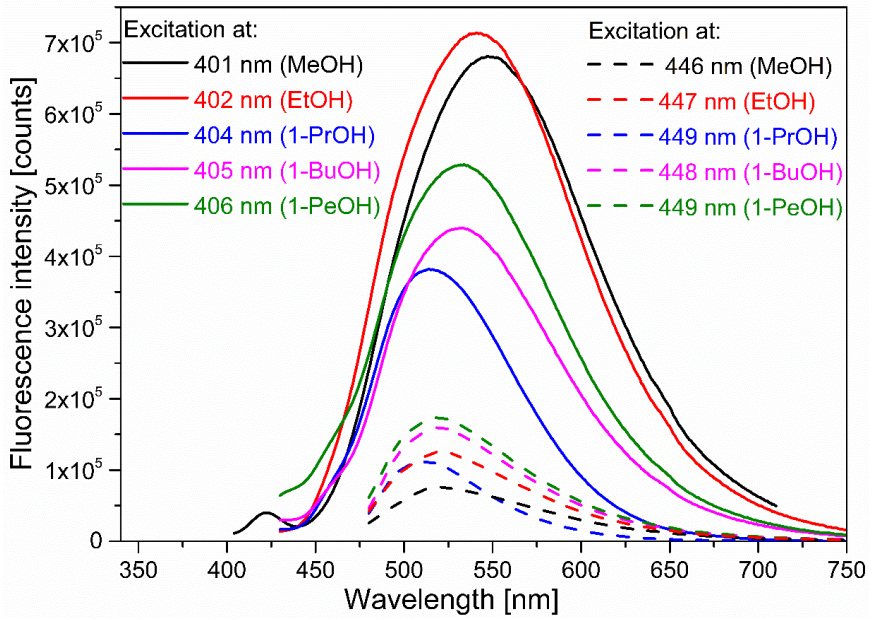


*Fig. S8. Steady-state emissions of **5** in alcohols obtained by excitation at ~ 400 nm (enol form) and at ~ 450 nm (keto tautomer) at concentration C_M ~ 6×10^{-6} mol L^{-1} .*

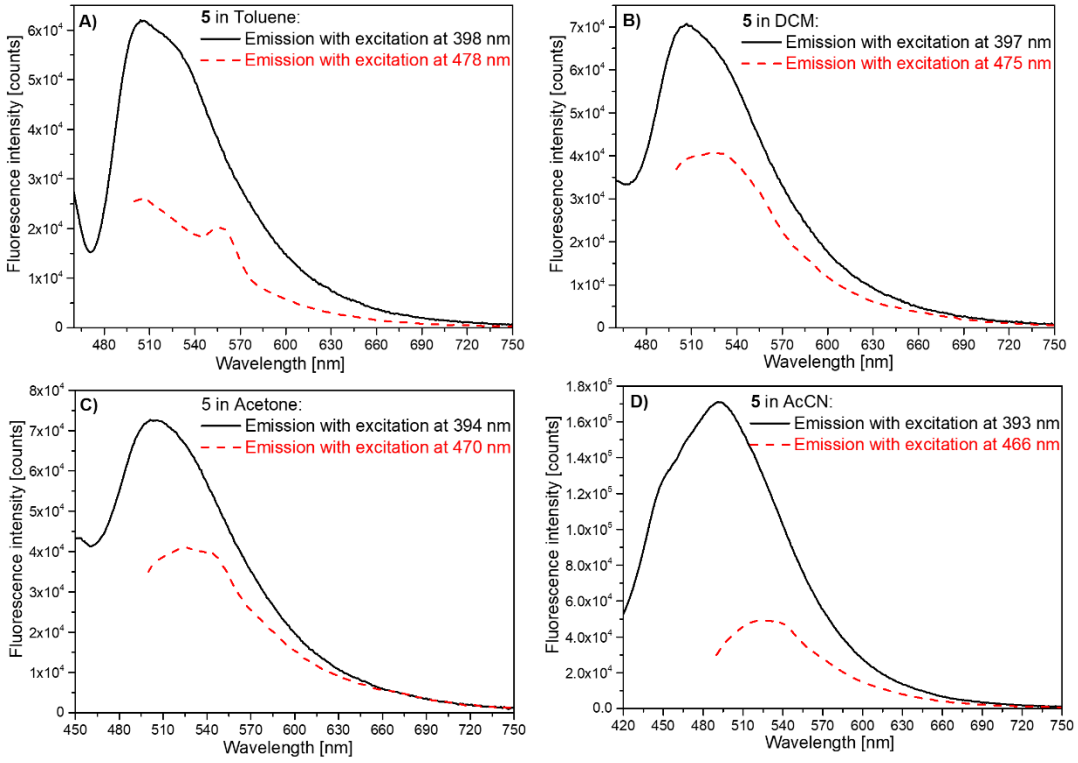


*Fig. S9. Steady-state emissions of **5** in various aprotic solvents with increasing polarity obtained by excitation at ~ 400 nm (enol form) and at ~ 470 nm (keto tautomer) at concentration C_M ~ 6×10^{-6} mol L^{-1}.*

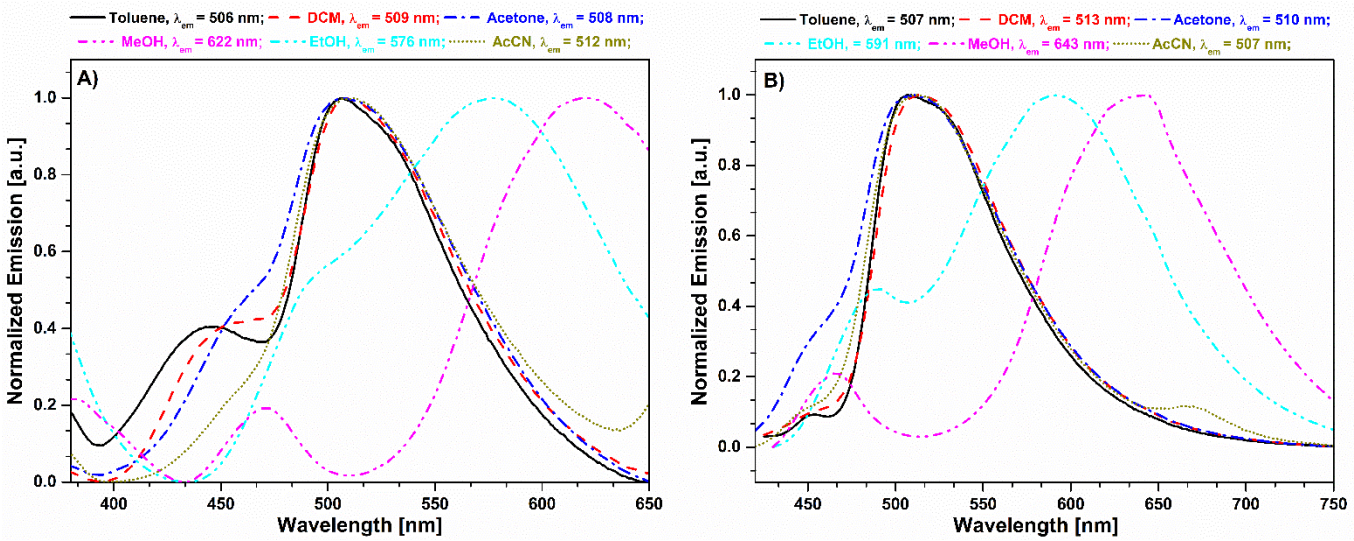
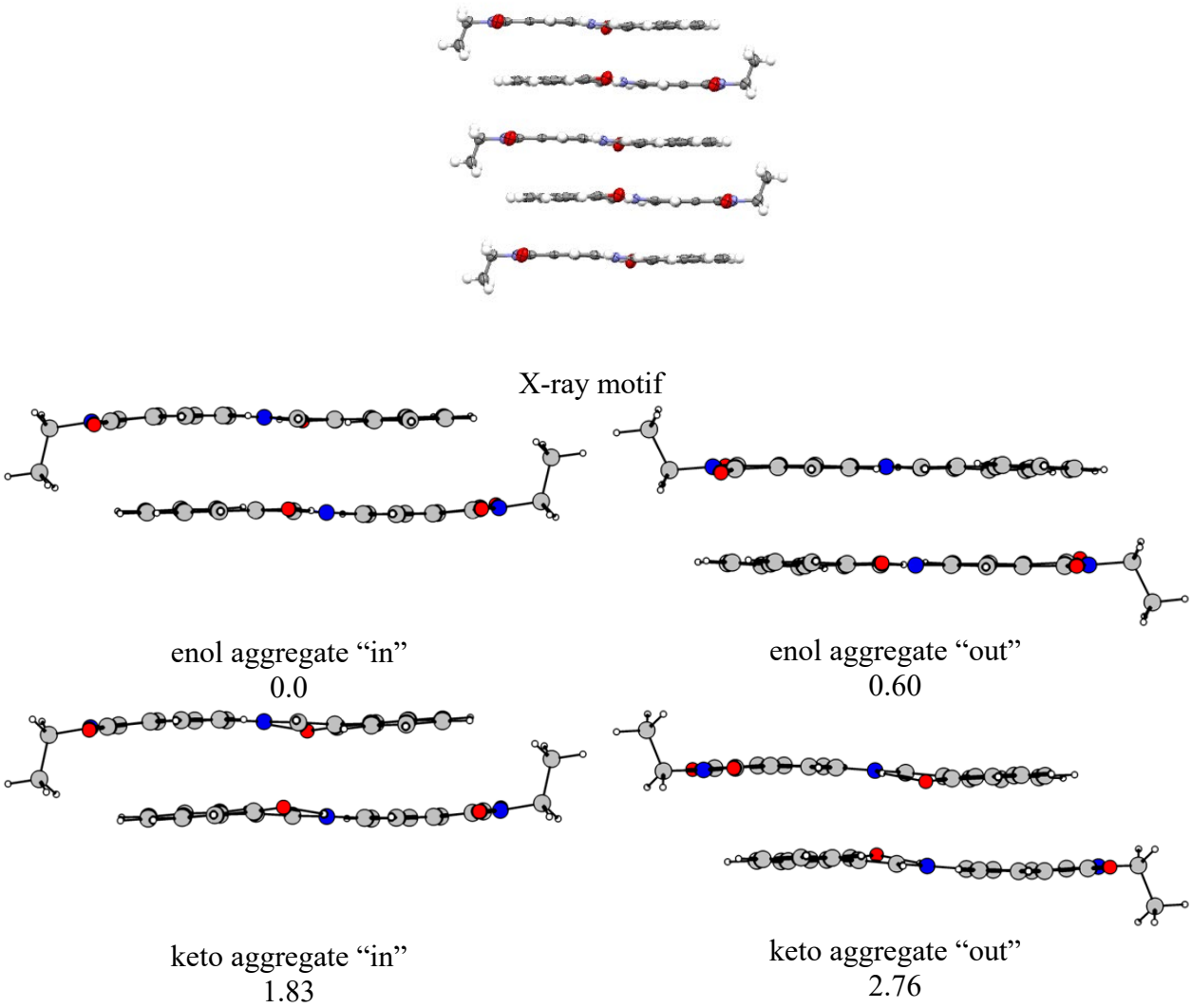


*Fig.S10. Steady-state emissions of **5** in the various aprotic and protic solvents, obtained by excitation at ~ 400 nm (A) and at ~ 450 nm (B) at concentration* $C_M \sim 6\times10^{-5}$ *mol* L^{-1}.



*Scheme S1. Possible aggregates of **5** according the crystallographic data and optimized dimers (with constrained planarity) along with its relative energies (BSSE corrected, in kcal/mol units) in gas phase.*